1-Dodecyl-2-methylpyridin-1-ium iodide
14402-22-3 | DTXSID60506018

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -43.8 °C

Global applicability domain: Inside

Local applicability domain index: 7.15e-01

Confidence level: 7.40e-01

Nearest Neighbors from the Training Set

Image not found
Benzenamine, N,N-dibutyl-
Measured: -32.2
Predicted: -41.2

Image not found
Benzenamine, N,N-diethyl-2-methyl-
Measured: -60.0
Predicted: -47.9

Image not found
N,N-Diethylaniline
Measured: -38.8
Predicted: -41.1

Image not found
Benzenamine, N,N,2,6-tetramethyl-
Measured: -36.0
Predicted: -40.5

Image not found
N,N,2-Trimethylaniline
Measured: -60.0
Predicted: -41.7